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Effect of g-jitter on directional solidification of a binary alloy

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Abstract

A study of directional solidification of a weak binary alloy (specifically, Bi - 1 at% Sn) based on the fixed grid single domain approach is being undertaken. The enthalpy method is used to solve for the temperature field over the computational domain including both the solid and liquid phases; latent heat evolution is treated with the aid of an effective specific heat coefficient. A source term accounting for the release of solute into the liquid during solidification has been incorporated into the solute transport equation. The vorticity-stream function formulation is used to describe thermo-solutal convection in the liquid region. In this paper we present a numerical simulation of g-jitter: the small, rapid fluctuations in gravitational acceleration which may be experienced in an orbiting space vehicle. A background gravity of 1 μg has been assumed, and new results for the effects of orientation angle of the periodic disturbances over a range of amplitudes and frequencies on solute field and segregation have been presented.

1 Introduction

The investigation of solidification and melting processes in low gravity conditions is of great practical importance for crystal growth techniques. The quality of single crystals grown from the melt strongly depends on growth morphology and on macro-segregation (non-uniformity in solute concentration) in solidified ingots caused by convective heat and mass transfer effects. A low gravity environment produces conditions in which convection is decreased to a level at which crystal growth is largely diffusion controlled. Residual accelerations in orbiting space vehicles are of the order of one to several hundred μg (where 1 μg = 9.81×10^{-6} ms^{-2}). For this reason, much effort has been expended in recent years in performing crystal growth experiments in the microgravity environment of a spacecraft in earth orbit. Such effects as compositional and kinetic supercooling, and the influence of convection on compositional distribution in the melt, have been investigated under microgravity.

However, gravity in an orbiting space vehicle may not be steady in either magnitude or direction. Perturbations to the anticipated steady microgravity environment may arise from, for example, crew actions, the operation of machinery and thruster rocket firings. Such perturbations are known as g-jitter.

The effects of gravity perturbations on the composition distribution in the Bridgman crystal growth configuration have been investigated numerically in a number of papers. Alexander, Ouazzani and Rosenberger [1] investigated the effects of steady and impulse residual acceleration on dopant distribution in Bridgman-Stockbarger crystal growth with different gravity vector orientations. It was found that lateral non-uniformity in composition, or segregation, is very sensitive to the orientation of the steady component of the residual gravity vector.

Transient and periodic accelerations have been considered by Alexander, Amiroudine, Ouazzani, and Rosenberger [2]. It was found that the largest compositional nonuniformities occur for disturbances with amplitudes above 10^{-6}g and frequencies below 10^{-2} Hz. At higher frequencies, larger acceleration amplitudes are required to obtain significant nonuniformities. Numerical results for the effect of g-jitter on the average interface concentration during Bridgman crystal growth in space are presented in Garandet, Corre, Favier and Alexander [3]. In all of these works a pseudo-steady-state model was adopted with the constraint that the interface is planar. This is a simplification of the true unsteady solidification process.

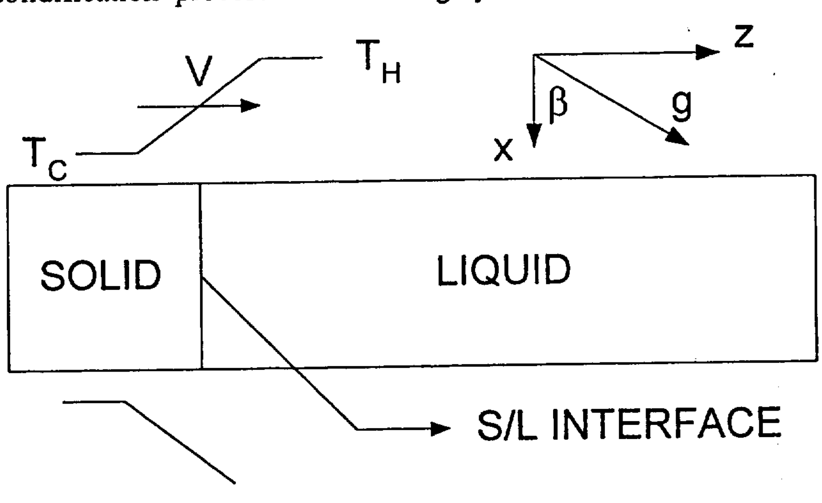
In actual growth situations, the solid-liquid interface can be non-planar due to thermal and mass transfer conditions and also due to morphological instability factors. A pseudo-steady-state model neglects transient effects such as changes in the velocity, temperature and concentration with time due to changes in the length of melt caused by translating the ampoule in which the solidifying material is contained. Investigation of solute redistribution during the initial transients becomes crucial for an alloy with a low partition coefficient solidifying at low rates because the steady state is difficult to reach in laboratory experiments.

In this work, we continue from previous work [4], for which the g-jitter and background gravity were always parallel to each other and orthogonal to the ampoule axis. In this paper, the effects of orientation of the periodic gravity perturbations, as well as those of amplitude and frequency, on segregation and solute distribution during transient directional solidification of Bi-1%Sn alloy in a Bridgman furnace have been investigated. A background gravity of 1 μg normal to the axis of the ampoule, which corresponds to a typical spacecraft environment, is considered.

2 Problem Definition

We consider a Bridgman furnace in which a moving temperature profile consisting of a cold zone (T_c), a nominally adiabatic zone and a hot zone (T_h) is imposed on the boundary of the ampoule. This boundary temperature profile is translated with a constant pulling velocity of 3.34 m s^{-1} as a result of the furnace movement causing the solid/liquid interface to move along the ampoule. The material in the ampoule is thus divided into two sub-regions: solid and liquid (see Figure 1). For the purpose of these computations, a distance of 5 mm has been initially solidified without g-jitter; the liquid zone is then 37 mm long. The ampoule is 6 mm in diameter.

Although the ampoule is three-dimensional, a two-dimensional model has been used. This simplification is valid because, under the microgravity conditions being considered, convection is very weak and the solidification process remains largely diffusion-controlled. Newtonian and



laminar flow is assumed in the liquid phase, and the Boussinesq approximation has been used, in which the liquid density is assumed to be constant except in the buoyancy term of the equation of motion. Details of the governing equations, boundary conditions, solution procedure, code validation and mesh independence validation were given by Benjapiyaporn *et al.* [4].

3. Results and Discussion

Simulations were undertaken for the directional solidification of a binary alloy (Bi/1at% Sn). The effects of orientation angle, amplitude and frequency of the disturbances have been studied. In the previous study [4], it was found that a small frequency and high amplitude of the disturbances will have an effect on the solidification process. As a result, the current studies were performed for amplitudes of 10^{-3}g and 10^{-2}g, and frequencies of 0.01Hz and 0.1Hz. The simulations were investigated for four different orientation angles (β): 0°, 45°, 90° and -45°.

Figure 2 shows the variations of the maximum transverse velocity u_x (wherever that occurs in the melt) with time for a disturbance of 10^{-3}g and 0.01Hz. As the orientation angle changes from 0° to 45°, 90° and -45°, u_x reduces. The 45° and -45° results are very close, and at 90° there is very little effect. A similar effect is found for the maximum longitudinal velocity u_z (not shown). Therefore, g-jitter induced convection becomes smaller as the orientation angle changes from 0° to other values.

Figure 3 shows the variation of u_z at the ampoule mid-height approximately at the centre of the melting zone. It is observed that changing the orientation angle from 0° to 45°, 90° and -45° *increases* u_z at the middle of the melting zone, in contrast to the effect on $u_{z|max}$. However, the variation of u_x at this location is similar to that shown in Figure 2.

As the magnitude of the gravity vector varies through its cycle, the flow in the ampoule oscillates between a clockwise and an anticlockwise circulation, except for = 90° for which the flow is more complex. Figure 4 shows velocity vectors for the four directions of g-jitter at the time in the cycle at which the velocity reaches a maximum. At = 90°, a flow is induced in the middle of the melting zone, much weaker than for the other angles and there is little effect in the region close to the interface. Figure 5 shows the variation of u_z at the ampoule mid-height at the end of the sample remote from the interface. It confirms that changes in the orientation angle have significant effects on the flow patterns in the sample.

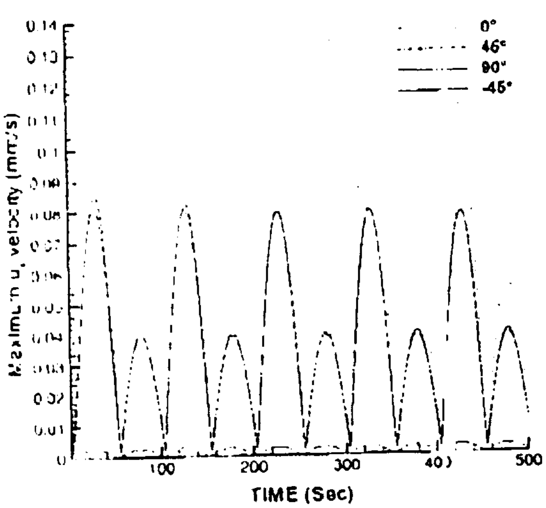


Figure 2 Variation of maximum u_x with time for the disturbance of 10^{-3}g and 0.01Hz.

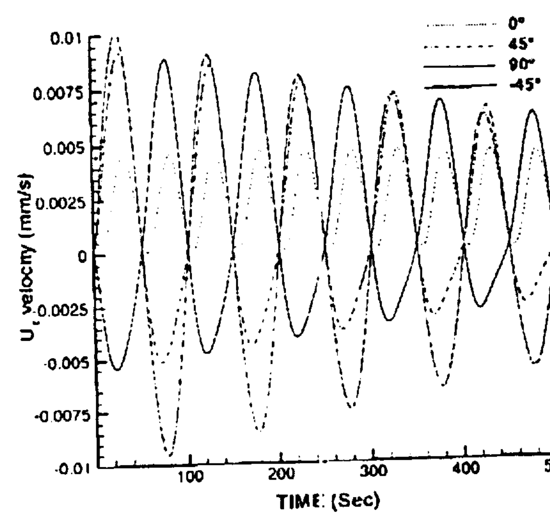


Figure 3 Variation of u_z at the mid-high at the centre of the melt with time for the disturbance of 10^{-3}g and 0.01Hz.

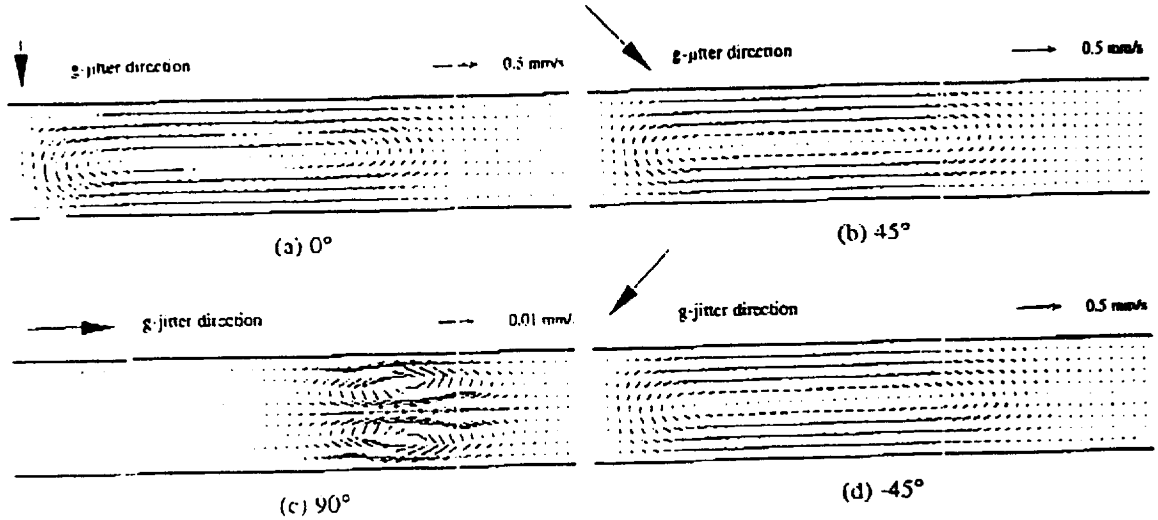


Figure 4 Velocity field at the peak of the disturbance of 10^{-3}g and 0.01Hz.

Figure 6 shows the variation with time of radial segregation in the solid at the interface for the same disturbance: 10^{-3}g and 0.01Hz, where $= (C_{max} - C_{min})/C_{ave}$ and C is the solute (*i.e.* Sn) concentration. For $\beta = 0°$, the disturbance induces a stronger flow close to the interface, which leads to higher segregation. At 90°, the disturbance has an effect on the flow at the middle of the melting zone far from the interface, but not near it; therefore there is almost no effect on the radial segregation at the interface. For $\beta = 45°$ and -45°, there are different transients of radial segregation during the first 500 seconds of the disturbance. However, at later times (not shown), the trend of the radial segregation is to become periodic and similar for the two angles.

Figure 7 shows the variation of radial segregation with time for a disturbance of 10^{-2}g and 0.01Hz. In [4], it was found that there is a strong convection in this case due to the very high amplitude and small frequency of the disturbance. The solute rich boundary layer in front of the interface is carried away and mixed into the melt. For $\beta = 0°$, 45° and -45°, the transients are different in the first approximately 300 seconds. After that time, the concentration field reaches the mixing stage and starts to have a periodic trend. At 90°, the radial segregation is not affected for the first 100 seconds, because the main circulation occurs at the middle of the melt far from the interface. During the second cycle of

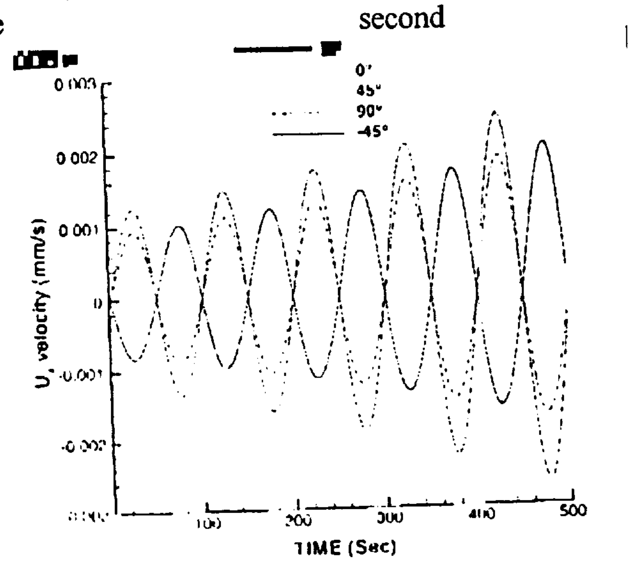


Figure 5 Variation of u_r at the mid-high at the end of the sample remote from the interface with time for the disturbance of 10^{-3}g and 0.01Hz.

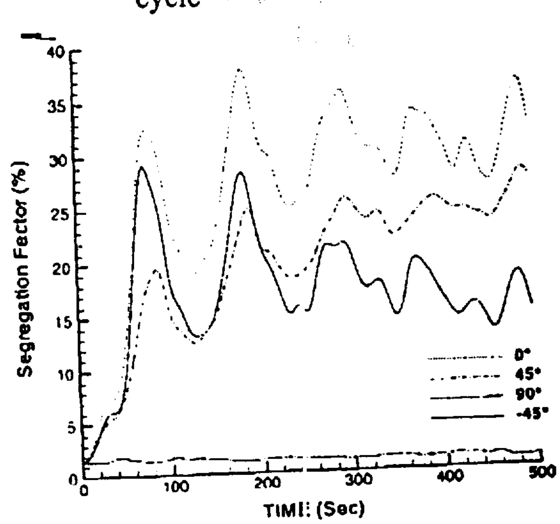


Figure 6 Variation of radial segregation with time for the disturbance of 10^{-3}g and 0.01Hz.

time for the disturbance of 10^{-3}g and 0.01Hz.

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disturbance of 10^{-3}g and 0.01Hz.

the disturbance, additional convection cells are formed just in front of the interface when the direction of the gravity vector points into the interface; these disappear when the direction of the gravity turns to the opposite direction. These cells become bigger until periodic behaviour is reached. The strength of the flow in the additional cells is stronger than that of the main circulation.

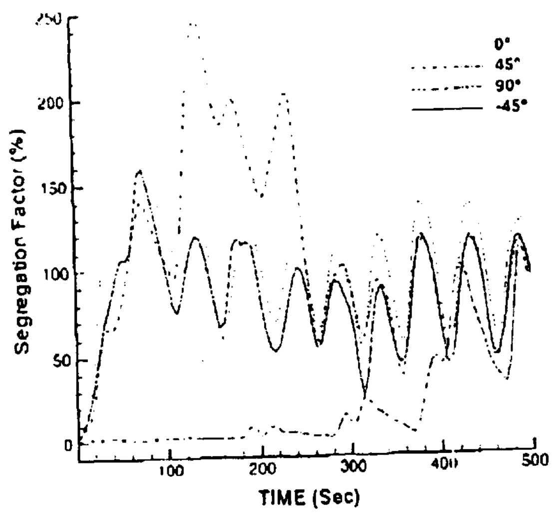


Figure 7 Variation of radial segregation with time for the disturbance of 10^{-2}g and 0.01Hz.

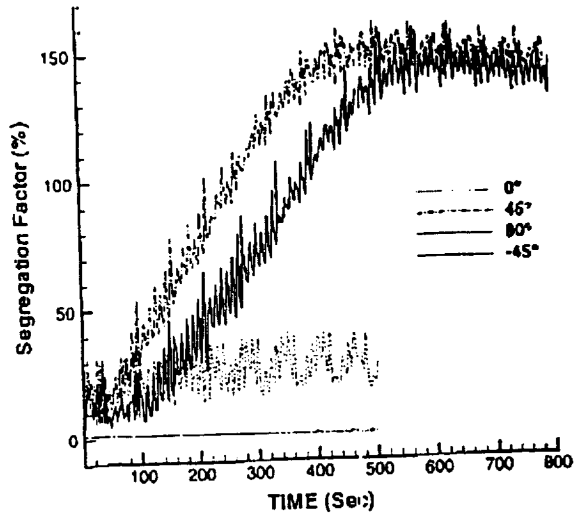
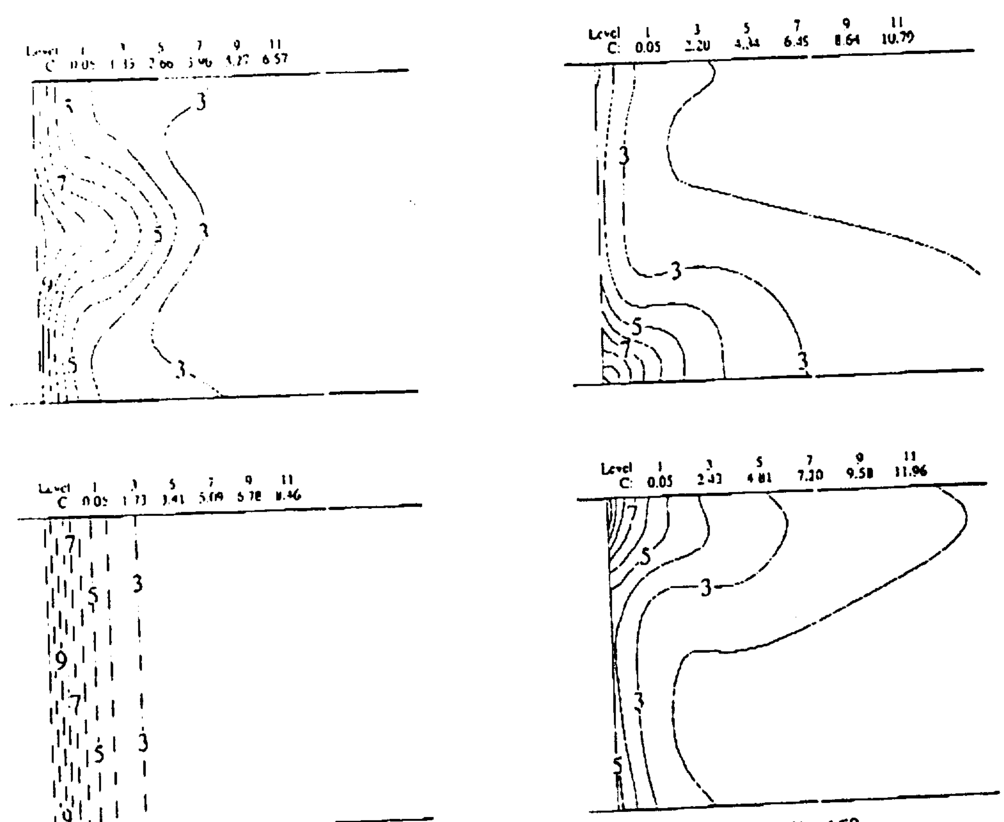


Figure 8 Variation of radial segregation with time for the disturbance of 10^{-2}g and 0.1Hz.



(c) 90°

(d) -45°

Figure 9 Contours of concentration for the disturbance of 10^{-2}g and 0.1Hz.

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Figure 8 shows the variation of radial segregation with time for 10^{-2}g and 0.1Hz. The strength of the flow reduces as the orientation angle changes from 0° to 45°, 90° and -45°. However, the radial segregation does not tend to follow the strength of the flow. The contours of concentration at a time when the fluctuating gravity passes through zero are shown in Figure 9. For $\beta = 0°$, the concentration field reaches the periodic stage about 100 s after the start of g-jitter. For $\beta = 45°$ and -45°, there are differences in the transient period (during first 500 seconds after the start of g-jitter). After the flow and concentration fields reach periodic behavior, the radial segregation factors converge to the same value, one which is much higher than that for $\beta = 0°$. Figures 9b and 9c confirm that the segregation is greater for $\beta = 45°$ and -45° than at 0°, even though the strength of convection is lower. At 90°, there is no effect from the disturbance on the concentration field.

4 Conclusions

We have investigated numerically the effects of sinusoidal disturbances with amplitudes from 10^{-3}g to 10^{-2}g, frequencies from 0.01 to 0.1 Hz and orientation angles of 0°, 45°, 90° and -45° on the solute redistribution and segregation at the interface during directional solidification of Bi-1at% Sn alloy. It was found that segregation not only depends on the strength of the flow field, but also depends on the flow character. Furthermore, the flow character strongly depends on the combination of orientation angle, amplitude and frequency of the disturbance.

References

[1] Alexander, J.I.D., Ouazzani, J., Rosenberger, F., 1989, Analysis of the low gravity tolerance of Bridgman-Stockbarger crystal growth: I. Steady and impulse accelerations, J. Crystal Growth, Vol. 97, pp. 285-302.

[2] Alexander, J.I.D., Amiroudine S., Ouazzani, J., Rosenberger, F., 1991, Analysis of the low gravity tolerance of Bridgman-Stockbarger crystal growth: II. Transient and periodic accelerations, J. Crystal Growth, Vol. 113, pp. 21-38.

[3] Garandet G.P., Corre S., Favier J.J. and Alexander, J.I.D, 1996, On the effect of gravity perturbations on composition profiles during Bridgman crystal growth in space, J. Crystal Growth, Vol. 165, pp. 471-481.

[4] Benjapiyaporn, C., Timchenko, V., de Vahl Davis, G., Leonardi, E. and de Groh III, H.C., 1998, Effects of g-jitter on directional solidification of binary alloy, IAF-98-J.2.01.